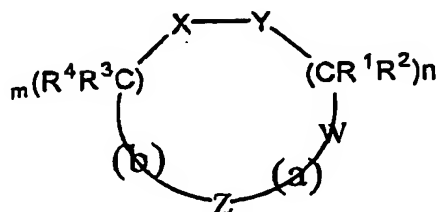


**CLAIMS:**

1. Scaffold-based compound having the following general formula (B):



(B)

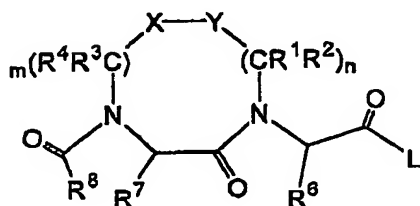
- including pharmaceutically acceptable salts, esters or solvates thereof,
- wherein
- Z is selected from C=O and -CH<sub>2</sub>-,
- W is selected from C=O and a bond, provided that at least one of Z and W is C=O,
- X and Y are independently selected from CH<sub>2</sub>, O, S, NH, N-R<sup>5</sup>, NH-CO, CO, CH<sub>2</sub>CO, S=O and SO<sub>2</sub>, or X and Y may form together a group selected from CH=CH, CO-NR<sup>5</sup>, NH-CO-NH, O-CH(R<sup>5</sup>)-O, NH-CH(R<sup>5</sup>)-O and NH-CH(R<sup>5</sup>)-NH, where the hydrogen in the above groups may optionally be substituted by an alkyl group,
- (a) and (b) are parts of the scaffold and are nitrogen containing bivalent organic radicals, each independently providing between 1 to 4 atoms to said scaffold,
- R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup> and R<sup>4</sup> are each independently selected from H and substituted or unsubstituted alkyl, and
- n and m are integers from 1 to 6, with the exclusion of the following compound: glycineamide, L-tyrosyl-N-[2-[(2S)-4-[(1S)-1-carboxy-3-methylbutyl]-3,4,5,8-tetrahydro-3-oxo-2-(phenylmethyl)-1,4-diazocin-1(2H)-yl]2-oxoethyl].
2. A compound of the formula (B) according to Claim 1, wherein X and Y are independently selected from CH<sub>2</sub>, O, S, NH, N-R<sup>5</sup>, NH-CO, CO, CH<sub>2</sub>CO, S=O and SO<sub>2</sub>, or X and Y may form together a group selected from CO-NR<sup>5</sup>,

NH-CO-NH, O-CH(R<sup>5</sup>)-O, NH-CH(R<sup>5</sup>)-O and NH-CH(R<sup>5</sup>)-NH, where the hydrogen in the above groups may optionally be substituted by an alkyl group.

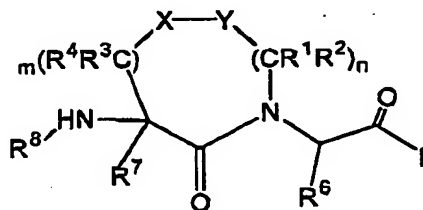
3. A compound according to Claim 1, with each of parts (a) and (b) providing up to two atoms to said scaffold.

4. A compound according to Claim 1, wherein each of parts (a) and (b) is independently selected from -N(CHR<sup>6</sup>COL)-, -C(COL)(R<sup>6</sup>)-, -N(COR<sup>8</sup>)-CHR<sup>7</sup>- and -C(NHR<sup>8</sup>)(R<sup>7</sup>)-.

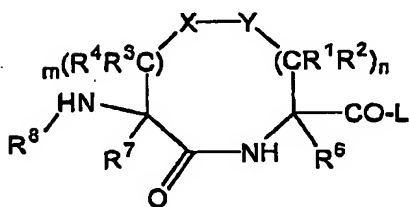
5. Compound of the formula I, II, III or IV:



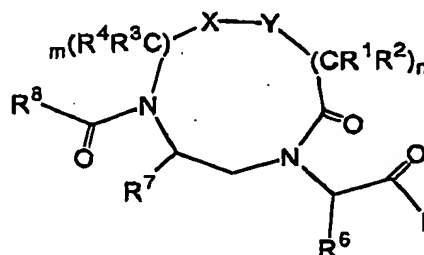
I



II



III



IV

including pharmaceutically acceptable salts, esters or solvates thereof, wherein

15 X and Y are independently selected from CH<sub>2</sub>, O, S, NH, N-R<sup>5</sup>, NH-CO, CO, CH<sub>2</sub>CO, S=O and SO<sub>2</sub>, or X and Y may form together a group selected from CH=CH, CO-NR<sup>5</sup>, NH-CO-NH, O-CH(R<sup>5</sup>)-O, NH-CH(R<sup>5</sup>)-O and NH-CH(R<sup>5</sup>)-NH, where the hydrogen in the above groups may optionally be

substituted by an alkyl group;  $R^1$ ,  $R^2$ ,  $R^3$  and  $R^4$  are each independently selected from H and substituted or unsubstituted alkyl;

$R^5$ ,  $R^6$ ,  $R^7$  and  $R^8$  are each independently selected from H, substituted or unsubstituted alkyl, cycloalkyl, aryl, aralkyl, hetroaryl, heterocyclyl, hetroaralkyl, acyl, carboxyaryl, carboxyalkyl, side chains of naturally and artificially occurring amino acids as well as derivatives and mimics of such side chains, and linear or cyclic peptide;

L is selected from H, OH,  $NH_2$ ,  $NHR^5$ , a peptide and a solid support, where  $R^5$  is as defined above, and

n and m are integers from 1 to 6, with the exclusion of the following compound: glycineamide, L-tyrosyl-N-[2-[(2S)-4-[(1S)-1-carboxy-3-methylbutyl]-3,4,5,8-tetrahydro-3-oxo-2-(phenylmethyl)-1,4-diazocin-1(2H)-yl]2-oxoethyl.

6. A compound of the formula I, II, III or IV according to Claim 5, wherein X and Y may form together a group selected from  $CO-NR^5$ ,  $NH-CO-NH$ ,  $O-CH(R^5)-O$ ,  $NH-CH(R^5)-O$  and  $NH-CH(R^5)-NH$ , where the hydrogen in the above groups may be substituted by an alkyl group.
7. A compound of the formula I, II, III or IV according to Claim 5, wherein X and Y form combinations selected from: both X and Y are S; X is NH and Y is CO; X is CO and Y is NH; X is NH and Y is  $CH_2$ ; X is  $CH_2$  and Y is NH; X and Y are  $NH-CO-NH$ ; X is  $N-R^4$  and Y is CO; and X is CO and Y is  $N-R^4$ .
8. A compound of the formula I according to Claim 5.
9. A compound of the formula II according to Claim 5.
10. A compound of the formula III according to Claim 5.
11. A compound of the formula IV according to claim 5.
12. A combinatorial library comprising a plurality of compounds of the formula (B) as defined in Claim 1.
13. A combinatorial library comprising a plurality of compounds of any one of the formulae I, II, III or IV as defined in Claim 5.

14. A library according to Claim 13, wherein in the compounds of the formulae I, II, III or IV, X and Y may form together a group selected from  $\text{CO-NR}^5$ ,  $\text{NH-CO-NH}$ ,  $\text{O-CH(R}^5\text{)-O}$ ,  $\text{NH-CH(R}^5\text{)-O}$  and  $\text{NH-CH(R}^5\text{)-NH}$ , where the hydrogen in the above groups may be substituted by an alkyl group.
15. A library according to Claim 13, wherein in the compounds of formulae I, II, III and IV, the following combinations for X and Y are selected from the group consisting of: (i) X and Y are both S; (ii) X is NH and Y is CO; (iii) X is CO and Y is NH; (iv) X is  $\text{N-R}^4$  and Y is CO; and (v) X is CO and Y is  $\text{N-R}^4$ .
16. A pharmaceutical composition comprising a pharmaceutically acceptable carrier and an effective amount of a compound of the formula I, II, III or IV as defined in Claim 5.
17. The composition of Claim 16 for the treatment of a disease, disorder or condition wherein a therapeutically beneficial effect is associated with the modulation of a protein or peptide-mediated cell activity.
18. A composition according to Claim 16 for use in veterinary.
19. A composition according to Claim 16 for use in human mammals.
20. A compound of formula I, II, III or IV as defined in Claim 5 for use in agriculture.
21. Use of a compound of the formula I, II, III or IV as defined in Claim 5, for the preparation of a pharmaceutical composition.
22. A method for modulating protein or peptide-mediated cell activity comprising contacting a cell component having said protein or peptide with an effective amount of a compound of formula I, II, III or IV as defined in Claim 5.
23. A method for the treatment of a disease, disorder or condition wherein a therapeutically beneficial effect is associated with the modulation of a protein or peptide-mediated cell activity, the method comprising administering to a subject in need of such treatment a therapeutically effective amount of a compound of formula I, II, III or IV as defined in Claim 5.

24. A method according to Claim 23 wherein said cell activity is selected from proliferation, differentiation, cellular shape alteration, cellular elongation, uptake of substances by cells secretion of substances, cellular metabolism, and expression of various proteins.
- ✓5 25. A method of identifying a candidate which modulates a protein or peptide-mediated cell activity, such method comprising:
- (a) identifying in said protein or peptide, a domain which is essential for said activity,
  - (b) identifying in said domain, pharmacophors essential for the activity,
  - (c) planning a combinatorial library of compounds having the formula I, II, III or IV as defined in Claim 5, wherein each such compound comprises at least two of the pharmacophors identified in step (b) above or mimics or derivatives of the pharmacophors, where each member of the library differs from the other by at least one of the following: i) the size of the ring; ii) the order in which the pharmacophors are arranged in the ring; iii) the chemical nature of the ring; iv) the chemical nature of the pharmacophors; v) the chirality of the linker between the ring and the pharmacophor; and vi) the chirality of the pharmacophor;
  - (d) synthesizing a plurality of compounds among the compounds of the combinatorial library planned in step (c);
  - (e) screening the compounds synthesized in step (d) for candidates that modulate said activity.
26. A method according to Claim 25, comprising the following step after step (c) and before step (d):
- (c1) virtually screening on a computer the compounds planned in step (b) to identify compounds with desirable 3D structures and selecting these compounds, and wherein step (d) comprises: synthesizing the selected compound of step (c1).
27. A method according to Claim 25 wherein said activity is selected from: proliferation, differentiation, cellular shape alteration, cellular elongation,

uptake of substances by cells, secretion of substances, cellular metabolism, and level of expression of various proteins.

28. A method for obtaining compounds which modulate protein or peptide-mediated cell activity, the method comprising:

- 5 (1) identifying the candidate compounds according to the method of Claim 25;
- (2) contacting the compounds identified in step (1) with a test assay for determining a protein or peptide-mediated cell activity;
- 10 (3) collecting those molecules which modulate a protein or peptide-mediated cell activity in a test assay as compared to the modulation in the same test assay in the absence of said compound, thereby obtaining modulators of said activity; and
- 15 (4) producing the compounds obtained in step (3).

29. A method according to Claim 28, wherein said activity is selected from proliferation, differentiation, cellular shape alteration, cellular elongation, uptake of substances by cells, secretion of substances, cellular metabolism, and expression of various proteins.

20 30. Modulator of a protein or peptide-mediated cell activity obtained by the method of Claim 28.

31. A method for modulating a protein or peptide-mediated cell activity, such method comprising contacting a cell whose activity is to be modulated with a modulator obtained by the method of Claim 28.

25 32. A compound of formula I, II, III or IV as defined in Claim 5, being linked either directly or through a linker to a marker for imaging or to a drug.

33. A compound according to Claim 32, linked to a marker for imaging.

34. A compound according to Claim 33 wherein the marker is for the detection of fluorescence, X-ray, MRI or radio-isotope scan.